



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:07 PM GMT

PDB ID : 1WDD  
Title : Crystal Structure of Activated Rice Rubisco Complexed with 2-Carboxyarabinitol-1,5-bisphosphate  
Authors : Mizohata, E.; Matsumura, H.; Ueno, T.; Ishida, H.; Inoue, T.; Makino, A.; Mae, T.; Kai, Y.  
Deposited on : 2004-05-13  
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

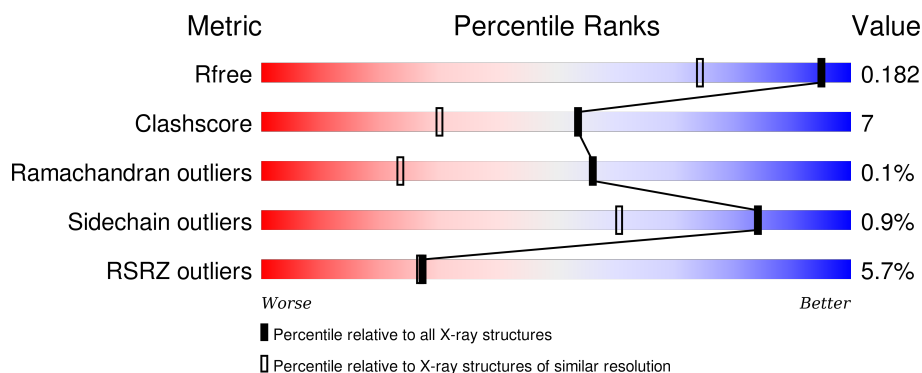
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2199 (1.40-1.32)
Clashscore	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	477	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>• •</div> </div>
1	E	477	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
2	S	128	<div> <div>16%</div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div>
2	W	128	<div> <div>10%</div> <div>73%</div> <div>23%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	3004	-	-	-	X
5	GOL	A	3006	-	-	-	X
5	GOL	A	3010	-	-	-	X
5	GOL	A	3015	-	-	X	X
5	GOL	E	3005	-	-	-	X
5	GOL	E	3009	-	-	-	X
5	GOL	E	3014	-	-	-	X
5	GOL	E	3016	-	-	X	X
5	GOL	W	3007	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10448 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3639	2311	639	669	20			
1	E	464	Total	C	N	O	S	0	0	0
			3632	2306	638	668	20			

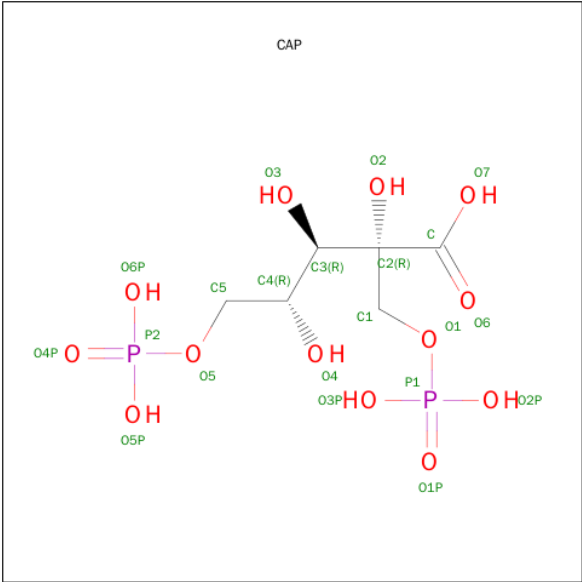
- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	122	Total	C	N	O	S	0	0	0
			1016	672	163	175	6			
2	W	122	Total	C	N	O	S	0	0	0
			1016	672	163	175	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

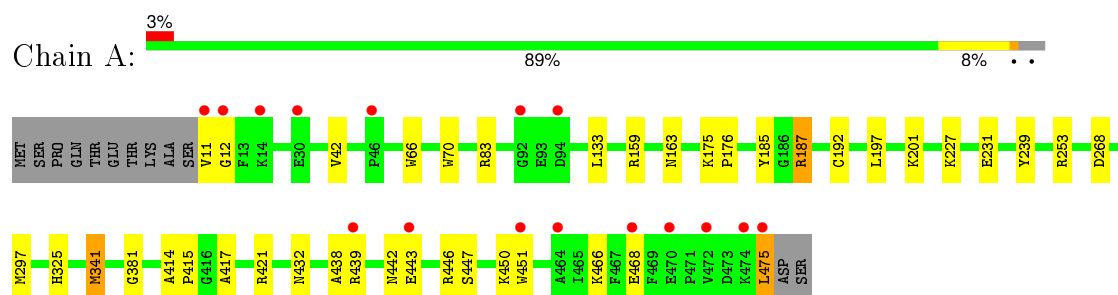
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	402	Total	O	0	0
			402	402		
6	E	366	Total	O	0	0
			366	366		
6	S	120	Total	O	0	0
			120	120		
6	W	111	Total	O	0	0
			111	111		

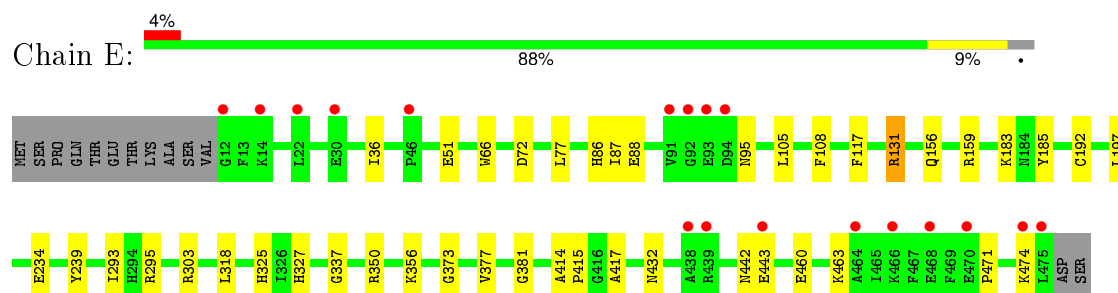
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

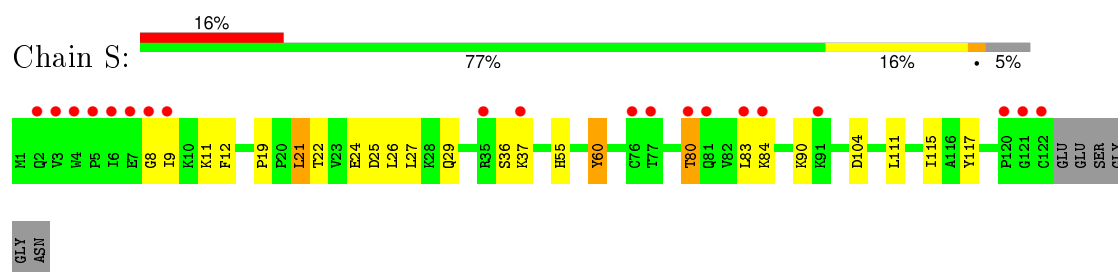
- Molecule 1: Ribulose biphosphate carboxylase large chain

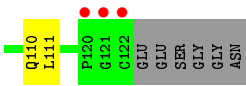


- Molecule 1: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase small chain C







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.71Å 111.71Å 196.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.32 – 1.35 22.32 – 1.36	Depositor EDS
% Data completeness (in resolution range)	98.3 (22.32-1.35) 98.5 (22.32-1.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 1.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.160 , 0.182 0.161 , 0.182	Depositor DCC
$R_{free}$ test set	12745 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 61.8	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 255778 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MME, GOL, MG, CAP, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.02	1/3717 (0.0%)	0.99	10/5035 (0.2%)
1	E	1.02	2/3710 (0.1%)	0.99	8/5025 (0.2%)
2	S	0.89	0/1039	0.88	0/1410
2	W	0.92	0/1039	0.94	0/1410
All	All	1.00	3/9505 (0.0%)	0.97	18/12880 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	MET	CG-SD	5.74	1.96	1.81
1	E	117	PHE	CD1-CE1	5.71	1.50	1.39
1	E	234	GLU	CB-CG	5.66	1.62	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	187	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	E	303	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	159	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	E	159	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	268	ASP	CB-CG-OD1	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	MET	CG-SD-CE	5.71	109.34	100.20
1	A	187	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	239	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	E	303	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	E	131	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	325	HIS	CB-CA-C	-5.41	99.57	110.40
1	A	421	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	350	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	83	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	159	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	E	159	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	325	HIS	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	60	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3639	0	3554	36	0
1	E	3632	0	3545	32	0
2	S	1016	0	1020	23	0
2	W	1016	0	1020	31	2
3	A	1	0	0	0	0
3	E	1	0	0	0	0
4	A	21	0	7	0	0
4	E	21	0	7	0	0
5	A	42	0	56	7	0
5	E	48	0	64	11	0
5	W	12	0	16	10	0
6	A	402	0	0	5	2
6	E	366	0	0	12	4
6	S	120	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	111	0	0	4	1
All	All	10448	0	9289	121	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:104:ASP:OD1	2:W:106:VAL:HG22	1.59	1.00
1:A:443:GLU:HG3	6:A:3143:HOH:O	1.73	0.88
1:E:356:LYS:NZ	6:E:3356:HOH:O	2.06	0.87
1:E:95:ASN:ND2	6:E:3315:HOH:O	2.09	0.85
5:A:3001:GOL:H12	6:A:3407:HOH:O	1.75	0.84
1:A:432:ASN:HD22	2:S:29:GLN:HE22	1.26	0.84
2:W:87:GLU:HG3	6:W:865:HOH:O	1.75	0.83
1:E:373:GLY:H	5:E:3016:GOL:C1	1.92	0.82
1:A:475:LEU:HD12	1:A:475:LEU:H	1.45	0.82
2:W:84:LYS:HE3	2:W:88:GLU:HG2	1.62	0.81
1:E:432:ASN:HD22	2:W:29:GLN:HE22	1.25	0.81
1:E:373:GLY:H	5:E:3016:GOL:H11	1.48	0.79
1:A:450:LYS:HD2	1:A:450:LYS:N	1.97	0.79
2:W:84:LYS:NZ	2:W:88:GLU:OE1	2.15	0.78
2:W:25:ASP:OD2	6:W:935:HOH:O	2.03	0.76
1:A:450:LYS:HD2	1:A:450:LYS:H	1.49	0.76
1:A:438:ALA:HB3	1:A:439:ARG:HH21	1.51	0.76
2:W:99:ARG:HH21	5:W:3007:GOL:H31	1.53	0.73
1:E:183:LYS:HE3	6:E:3112:HOH:O	1.87	0.73
1:A:11:VAL:HG12	1:A:12:GLY:N	2.04	0.72
1:E:443:GLU:HG3	6:E:3161:HOH:O	1.88	0.71
2:S:25:ASP:OD2	6:S:192:HOH:O	2.10	0.70
5:A:3001:GOL:C1	6:A:3407:HOH:O	2.38	0.68
1:E:156:GLN:OE1	5:E:3016:GOL:H12	1.96	0.66
5:E:3002:GOL:O1	6:E:3375:HOH:O	2.10	0.65
2:W:84:LYS:HE3	2:W:88:GLU:CG	2.25	0.65
1:A:466:LYS:HG3	1:A:468:GLU:HG3	1.79	0.65
1:A:451:TRP:CD2	2:S:19:PRO:HG3	2.31	0.65
2:S:80:THR:HA	2:S:83:LEU:HD12	1.78	0.65
1:A:466:LYS:HD2	6:A:3149:HOH:O	1.96	0.64
1:E:295:ARG:HH12	5:E:3014:GOL:H31	1.63	0.64
1:A:70:TRP:HA	5:A:3012:GOL:H32	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:C	1:A:450:LYS:HZ2	2.01	0.63
5:E:3009:GOL:H12	6:E:3366:HOH:O	1.98	0.63
1:E:460:GLU:CG	6:E:3374:HOH:O	2.47	0.62
2:W:43:GLU:OE2	5:W:3007:GOL:H12	2.01	0.61
1:E:460:GLU:HG3	6:E:3374:HOH:O	2.01	0.61
2:S:84:LYS:HE3	6:S:223:HOH:O	2.01	0.61
1:E:131:ARG:HD2	6:E:3377:HOH:O	2.01	0.60
2:S:12:PHE:HB3	2:S:115:ILE:HG13	1.83	0.60
2:W:99:ARG:HH21	5:W:3007:GOL:C3	2.15	0.60
1:A:42:VAL:HG22	1:A:133:LEU:CD1	2.33	0.59
2:S:12:PHE:CB	2:S:115:ILE:HG13	2.33	0.59
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.83	0.59
1:E:373:GLY:N	5:E:3016:GOL:H11	2.16	0.59
2:S:21:LEU:HD23	2:S:26:LEU:HD23	1.84	0.59
1:A:11:VAL:CG1	1:A:12:GLY:N	2.66	0.58
2:W:50:VAL:CG2	2:W:61:TYR:HB3	2.34	0.58
1:E:156:GLN:OE1	5:E:3016:GOL:C1	2.53	0.56
2:S:9:ILE:HG22	2:S:11:LYS:HE2	1.88	0.55
1:E:460:GLU:CD	6:E:3374:HOH:O	2.44	0.55
2:W:43:GLU:OE1	5:W:3007:GOL:H31	2.08	0.54
2:S:27:LEU:HG	2:S:83:LEU:HD11	1.88	0.54
2:S:22:THR:OG1	2:S:24:GLU:HG3	2.08	0.53
2:W:27:LEU:O	2:W:31:GLU:HG3	2.09	0.53
1:A:187:ARG:HH22	5:A:3015:GOL:H11	1.74	0.53
2:W:110:GLN:OE1	5:W:3007:GOL:H11	2.09	0.52
1:A:11:VAL:CG1	1:A:12:GLY:H	2.23	0.52
2:W:66:TRP:H	5:W:3007:GOL:C3	2.24	0.51
2:W:50:VAL:HG23	2:W:62:ASP:O	2.10	0.51
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.92	0.51
2:S:90:LYS:HE3	2:S:117:TYR:CD1	2.44	0.51
2:W:65:TYR:HA	5:W:3007:GOL:H32	1.93	0.51
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.91	0.51
2:W:73:MET:CE	2:W:81:GLN:HE21	2.24	0.51
2:W:41:CYS:HB3	2:W:101:ILE:HD11	1.93	0.50
2:W:106:VAL:HG23	2:W:107:ARG:N	2.26	0.50
2:W:66:TRP:H	5:W:3007:GOL:H32	1.77	0.50
2:S:8:GLY:O	2:S:9:ILE:HD13	2.12	0.49
2:S:9:ILE:HG22	2:S:9:ILE:O	2.13	0.49
1:A:450:LYS:CD	1:A:450:LYS:H	2.20	0.48
1:A:187:ARG:HH22	5:A:3015:GOL:C1	2.26	0.48
2:W:38:TRP:CE2	2:W:111:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:101:ILE:HD12	2:W:101:ILE:C	2.33	0.48
1:A:438:ALA:CB	1:A:439:ARG:HH21	2.24	0.48
2:S:104:ASP:HB2	2:S:111:LEU:CD1	2.44	0.47
1:A:447:SER:O	1:A:450:LYS:HD3	2.15	0.47
1:E:295:ARG:HH12	5:E:3014:GOL:C3	2.28	0.47
2:W:106:VAL:CG2	6:W:749:HOH:O	2.63	0.47
2:W:50:VAL:HG22	2:W:51:TYR:N	2.29	0.47
1:A:475:LEU:HD12	1:A:475:LEU:N	2.22	0.47
1:A:11:VAL:HG12	1:A:12:GLY:H	1.74	0.47
1:A:187:ARG:NH2	5:A:3015:GOL:C1	2.79	0.46
2:S:21:LEU:HD23	2:S:26:LEU:CD2	2.46	0.46
1:A:381:GLY:HA2	1:E:66:TRP:CD1	2.51	0.46
1:E:86:HIS:HE1	1:E:88:GLU:OE1	1.99	0.46
2:W:50:VAL:HG23	2:W:61:TYR:HB3	1.98	0.45
2:W:106:VAL:HG21	6:W:749:HOH:O	2.16	0.45
2:W:73:MET:HE3	2:W:81:GLN:HE21	1.81	0.45
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.99	0.45
2:S:27:LEU:CD1	2:S:83:LEU:HD11	2.47	0.44
1:A:442:ASN:O	1:A:446:ARG:HG3	2.18	0.44
1:E:327:HIS:HA	1:E:377:VAL:HB	1.99	0.44
1:A:187:ARG:NH1	6:A:3271:HOH:O	2.50	0.43
1:E:36:ILE:HD12	1:E:108:PHE:CE2	2.54	0.43
1:A:201:KCX:HB2	1:A:239:TYR:CD2	2.54	0.43
2:W:99:ARG:NH2	5:W:3007:GOL:C3	2.80	0.43
1:E:192:CYS:HB3	1:E:197:LEU:HD12	2.00	0.42
1:E:51:GLU:HA	1:E:87:ILE:CD1	2.49	0.42
1:E:105:LEU:HB3	5:E:3002:GOL:H32	2.01	0.42
2:S:84:LYS:CE	6:S:223:HOH:O	2.65	0.42
2:S:12:PHE:HB3	2:S:115:ILE:CG1	2.49	0.42
1:E:72:ASP:HB2	5:E:3013:GOL:H12	2.02	0.42
1:A:175:LYS:HA	1:A:176:PRO:C	2.40	0.42
1:E:460:GLU:OE1	1:E:463:LYS:NZ	2.47	0.42
1:A:187:ARG:NH2	5:A:3015:GOL:H12	2.35	0.41
2:S:104:ASP:HB2	2:S:111:LEU:HD12	2.01	0.41
2:S:36:SER:O	2:S:37:LYS:HB2	2.20	0.41
1:A:66:TRP:CD1	1:E:381:GLY:HA2	2.56	0.41
2:W:38:TRP:NE1	2:W:111:LEU:HD12	2.35	0.41
2:W:43:GLU:CD	5:W:3007:GOL:H12	2.41	0.41
2:S:90:LYS:HG2	2:S:117:TYR:CG	2.56	0.41
1:A:447:SER:HA	1:A:450:LYS:NZ	2.36	0.40
1:A:414:ALA:HB3	1:A:415:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ILE:HG13	1:E:318:LEU:HD21	2.03	0.40
1:E:471:PRO:O	1:E:474:LYS:HE2	2.21	0.40
1:A:341:MET:CG	1:A:475:LEU:HG	2.52	0.40
1:A:227:LYS:O	1:A:231:GLU:HG3	2.21	0.40
1:E:131:ARG:CD	6:E:3377:HOH:O	2.67	0.40
2:S:60:TYR:C	2:S:60:TYR:CD1	2.95	0.40
1:E:442:ASN:ND2	6:E:3379:HOH:O	2.54	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:7:GLU:OE1	2:W:46:LYS:NZ[4_565]	1.91	0.29
6:A:3321:HOH:O	6:E:3375:HOH:O[4_565]	1.94	0.26
6:E:3249:HOH:O	6:E:3352:HOH:O[4_565]	2.02	0.18
2:W:24:GLU:OE2	6:S:192:HOH:O[6_555]	2.08	0.12
6:E:3320:HOH:O	6:W:693:HOH:O[4_565]	2.10	0.10
6:A:3266:HOH:O	6:E:3363:HOH:O[3_555]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/477 (97%)	448 (97%)	14 (3%)	0	100	100
1	E	461/477 (97%)	447 (97%)	13 (3%)	1 (0%)	52	22
2	S	120/128 (94%)	115 (96%)	5 (4%)	0	100	100
2	W	120/128 (94%)	114 (95%)	6 (5%)	0	100	100
All	All	1163/1210 (96%)	1124 (97%)	38 (3%)	1 (0%)	56	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	337	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/385 (97%)	371 (99%)	3 (1%)	86	65
1	E	373/385 (97%)	371 (100%)	2 (0%)	92	77
2	S	109/113 (96%)	106 (97%)	3 (3%)	51	14
2	W	109/113 (96%)	108 (99%)	1 (1%)	84	61
All	All	965/996 (97%)	956 (99%)	9 (1%)	84	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	185	TYR
1	A	475	LEU
2	S	21	LEU
2	S	55	HIS
2	S	80	THR
1	E	77	LEU
1	E	185	TYR
2	W	55	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	GLN
2	S	29	GLN
1	E	86	HIS
1	E	95	ASN
1	E	304	GLN
1	E	401	GLN
1	E	442	ASN

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Mol	Chain	Res	Type
2	W	29	GLN
2	W	81	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	A	201	1,3	7,11,12	0.79	0	7,12,14	0.98	0
1	KCX	E	201	1,3	7,11,12	1.46	2 (28%)	7,12,14	0.84	0
2	MME	S	1	2	7,8,9	1.78	1 (14%)	4,8,10	0.97	0
2	MME	W	1	2	7,8,9	1.78	1 (14%)	4,8,10	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
2	MME	S	1	2	-	0/4/8/10	0/0/0/0
2	MME	W	1	2	-	0/4/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	MME	CM-N	-4.61	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	1	MME	CM-N	-4.51	1.34	1.46
1	E	201	KCX	CE-NZ	2.40	1.51	1.46
1	E	201	KCX	CB-CA	2.80	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	KCX	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	CAP	A	1001	3	14,20,20	0.87	1 (7%)	15,31,31	1.05	0
5	GOL	A	3001	-	5,5,5	1.65	1 (20%)	5,5,5	1.07	0
5	GOL	A	3004	-	5,5,5	1.37	1 (20%)	5,5,5	0.47	0
5	GOL	A	3006	-	5,5,5	0.89	0	5,5,5	0.39	0
5	GOL	A	3010	-	5,5,5	1.05	0	5,5,5	0.48	0
5	GOL	A	3012	-	5,5,5	0.94	0	5,5,5	0.30	0
5	GOL	A	3015	-	5,5,5	1.25	1 (20%)	5,5,5	0.34	0
5	GOL	A	3017	-	5,5,5	0.77	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAP	E	2001	3	14,20,20	0.78	0	15,31,31	0.86	0
5	GOL	E	3002	-	5,5,5	1.20	0	5,5,5	0.97	0
5	GOL	E	3003	-	5,5,5	2.16	1 (20%)	5,5,5	0.98	1 (20%)
5	GOL	E	3005	-	5,5,5	1.03	0	5,5,5	0.44	0
5	GOL	E	3009	-	5,5,5	1.05	0	5,5,5	0.96	0
5	GOL	E	3011	-	5,5,5	1.44	1 (20%)	5,5,5	0.37	0
5	GOL	E	3013	-	5,5,5	0.96	0	5,5,5	0.45	0
5	GOL	E	3014	-	5,5,5	1.20	1 (20%)	5,5,5	0.81	0
5	GOL	E	3016	-	5,5,5	1.29	0	5,5,5	0.66	0
5	GOL	W	3007	-	5,5,5	1.04	0	5,5,5	0.30	0
5	GOL	W	3008	-	5,5,5	1.15	0	5,5,5	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	A	1001	3	-	0/23/29/29	0/0/0/0
5	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3004	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3006	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3010	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3012	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3015	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3017	-	-	0/4/4/4	0/0/0/0
4	CAP	E	2001	3	-	0/23/29/29	0/0/0/0
5	GOL	E	3002	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3003	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3005	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3009	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3011	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3013	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3014	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3016	-	-	0/4/4/4	0/0/0/0
5	GOL	W	3007	-	-	0/4/4/4	0/0/0/0
5	GOL	W	3008	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3001	GOL	C3-C2	-3.08	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3015	GOL	C3-C2	-2.23	1.43	1.52
4	A	1001	CAP	O2-C2	2.09	1.46	1.43
5	E	3014	GOL	O3-C3	2.33	1.52	1.42
5	A	3004	GOL	O3-C3	2.35	1.52	1.42
5	E	3011	GOL	O3-C3	2.68	1.53	1.42
5	E	3003	GOL	O3-C3	4.17	1.60	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3003	GOL	C3-C2-C1	2.13	119.49	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3001	GOL	2	0
5	A	3012	GOL	1	0
5	A	3015	GOL	4	0
5	E	3002	GOL	2	0
5	E	3009	GOL	1	0
5	E	3013	GOL	1	0
5	E	3014	GOL	2	0
5	E	3016	GOL	5	0
5	W	3007	GOL	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	464/477 (97%)	-0.19	16 (3%) 49 49	11, 16, 31, 46	0
1	E	463/477 (97%)	-0.20	18 (3%) 43 44	11, 15, 30, 49	0
2	S	121/128 (94%)	0.97	20 (16%) 2 3	13, 26, 40, 63	0
2	W	121/128 (94%)	0.62	13 (10%) 8 8	13, 25, 37, 66	0
All	All	1169/1210 (96%)	0.01	67 (5%) 27 27	11, 17, 35, 66	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	122	CYS	12.1
2	S	122	CYS	12.0
2	W	121	GLY	11.6
2	S	121	GLY	10.8
1	A	11	VAL	10.3
1	A	475	LEU	8.7
2	S	120	PRO	8.0
2	S	9	ILE	8.0
2	S	8	GLY	7.4
1	E	94	ASP	6.6
1	E	91	VAL	6.2
2	S	77	THR	5.9
2	W	120	PRO	5.7
1	E	475	LEU	5.5
2	W	8	GLY	5.4
1	E	439	ARG	5.1
2	S	6	ILE	4.9
1	E	92	GLY	4.8
1	A	451	TRP	4.7
1	A	470	GLU	4.6
2	W	9	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	4.3
1	E	12	GLY	4.1
1	A	439	ARG	4.1
2	W	77	THR	4.1
1	A	12	GLY	4.0
2	S	7	GLU	4.0
1	E	470	GLU	3.9
2	W	3	VAL	3.8
2	S	83	LEU	3.8
2	S	81	GLN	3.7
2	W	7	GLU	3.6
1	E	14	LYS	3.3
2	S	3	VAL	3.1
2	S	2	GLN	3.1
1	A	464	ALA	3.1
2	W	2	GLN	3.0
1	E	464	ALA	3.0
2	S	4	TRP	2.9
2	S	5	PRO	2.8
1	E	30	GLU	2.8
1	A	92	GLY	2.8
1	E	22	LEU	2.7
1	A	46	PRO	2.7
2	S	84	LYS	2.6
2	W	91	LYS	2.6
1	A	30	GLU	2.6
2	S	76	CYS	2.6
2	S	91	LYS	2.6
1	E	468	GLU	2.5
1	A	443	GLU	2.5
1	A	468	GLU	2.4
1	A	14	LYS	2.4
1	E	93	GLU	2.4
1	E	474	LYS	2.4
2	S	80	THR	2.4
2	W	5	PRO	2.4
2	W	80	THR	2.4
2	S	35	ARG	2.3
1	E	466	LYS	2.2
1	E	443	GLU	2.2
2	S	37	LYS	2.2
1	E	438	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	2.1
2	W	84	LYS	2.1
1	E	46	PRO	2.0
1	A	474	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	E	201	12/13	0.98	0.05	-	12,13,14,14	0
2	MME	S	1	9/10	0.90	0.20	-	36,40,47,48	0
1	KCX	A	201	12/13	0.99	0.04	-	11,12,13,13	0
2	MME	W	1	9/10	0.89	0.20	-	35,38,44,45	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	E	3014	6/6	0.71	0.17	10.04	32,37,40,40	0
5	GOL	E	3016	6/6	0.80	0.18	6.84	32,41,41,44	0
5	GOL	A	3015	6/6	0.86	0.16	5.21	30,37,40,45	0
5	GOL	A	3006	6/6	0.80	0.15	4.59	26,37,39,45	0
5	GOL	W	3007	6/6	0.91	0.12	3.86	23,33,34,39	0
5	GOL	A	3010	6/6	0.73	0.13	3.83	43,45,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	E	3009	6/6	0.79	0.14	3.69	39,41,43,43	0
5	GOL	A	3004	6/6	0.82	0.11	3.10	26,27,32,34	0
5	GOL	E	3005	6/6	0.87	0.10	2.23	24,33,35,40	0
5	GOL	W	3008	6/6	0.71	0.22	1.31	41,47,48,51	0
5	GOL	E	3002	6/6	0.88	0.09	1.23	30,34,35,38	0
5	GOL	A	3001	6/6	0.89	0.09	1.21	28,32,37,39	0
5	GOL	E	3011	6/6	0.90	0.09	1.14	27,28,32,35	0
5	GOL	E	3003	6/6	0.94	0.07	0.39	17,20,22,24	0
5	GOL	A	3012	6/6	0.87	0.15	0.34	49,51,52,53	0
5	GOL	E	3013	6/6	0.82	0.10	0.24	43,49,49,49	0
4	CAP	E	2001	21/21	0.99	0.04	-1.24	13,14,16,18	0
4	CAP	A	1001	21/21	0.99	0.04	-1.45	13,14,15,18	0
3	MG	A	1476	1/1	1.00	0.03	-2.59	13,13,13,13	0
3	MG	E	2476	1/1	1.00	0.03	-2.92	12,12,12,12	0
5	GOL	A	3017	6/6	0.83	0.22	-	32,42,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.